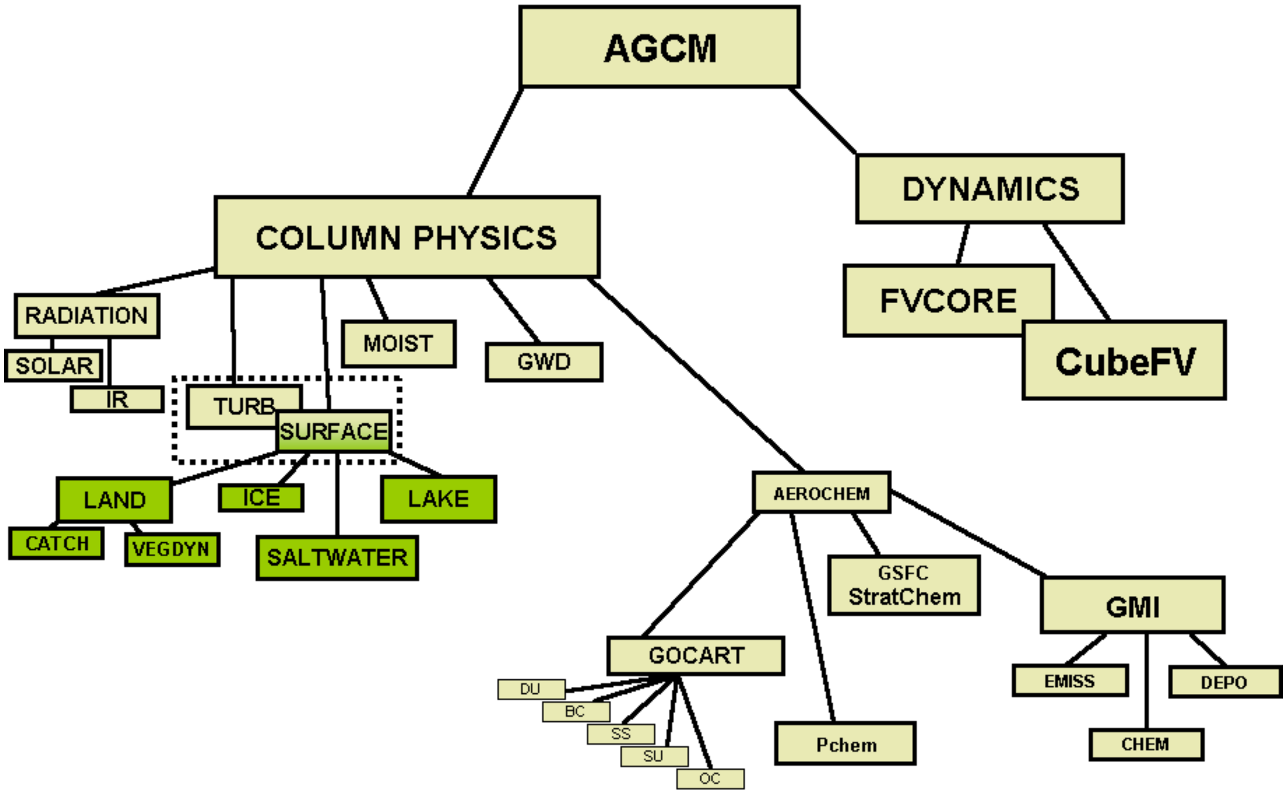
Progress in Adapting the GEOS-5 GCM to CUDA Fortran: Successes and Challenges

Matt Thompson

GEOS-5 GCM

- Goddard Earth Observing System Model, Version 5
  - Includes a Data Assimilation System (DAS)
    - Integrates the Global Climate System (GCM) with Gridpoint Statistical Interpolation (GSI)
- Focusing here on the Atmospheric GCM (AGCM)
  - Hierarchy of ESMF Gridded Components connected via MAPL

GEOS-5 GCM



AGCM
DYNAMICS
COLUMN PHYSICS
FVCORE
CubeFV
RADIATION
SOLAR
IR
MOIST
GWD
TURB
SURFACE
LAND
ICE
LAKE
CATCH
VEGDYN
SALTWATER
AEROCHEM
GSFC StratChem
GMI
GOCART
Pchem
EMISS
DEPO
CHEM
DU
BC
SS
SU
OC

GPU Conversion Aims

- Preserve bit-identical results on CPU whenever possible
- Minimize disruption to end-users
  - Checkout, build, etc. should look the same
  - GPU code a compile-time decision with a flag

GPU Conversion Method

- Current Host Code Layout
  - `#ifdef _CUDA`
    - Allocate Device Memory
    - Memory Copies to Device
    - Call GPU Kernels
    - Memory Copies to Host
    - Deallocate Device Memory
  - `#else`
    - Call CPU Kernel
  - `#endif`
- Don't duplicate code!
  - There is no irrad_gpu and irrad_cpu, only irrad!

GPU Conversion Method

- Device (aka "Kernel") Code Layout
  - Declare device & constant arrays (in module, use'd on host)
  - `attributes(global)` main routine

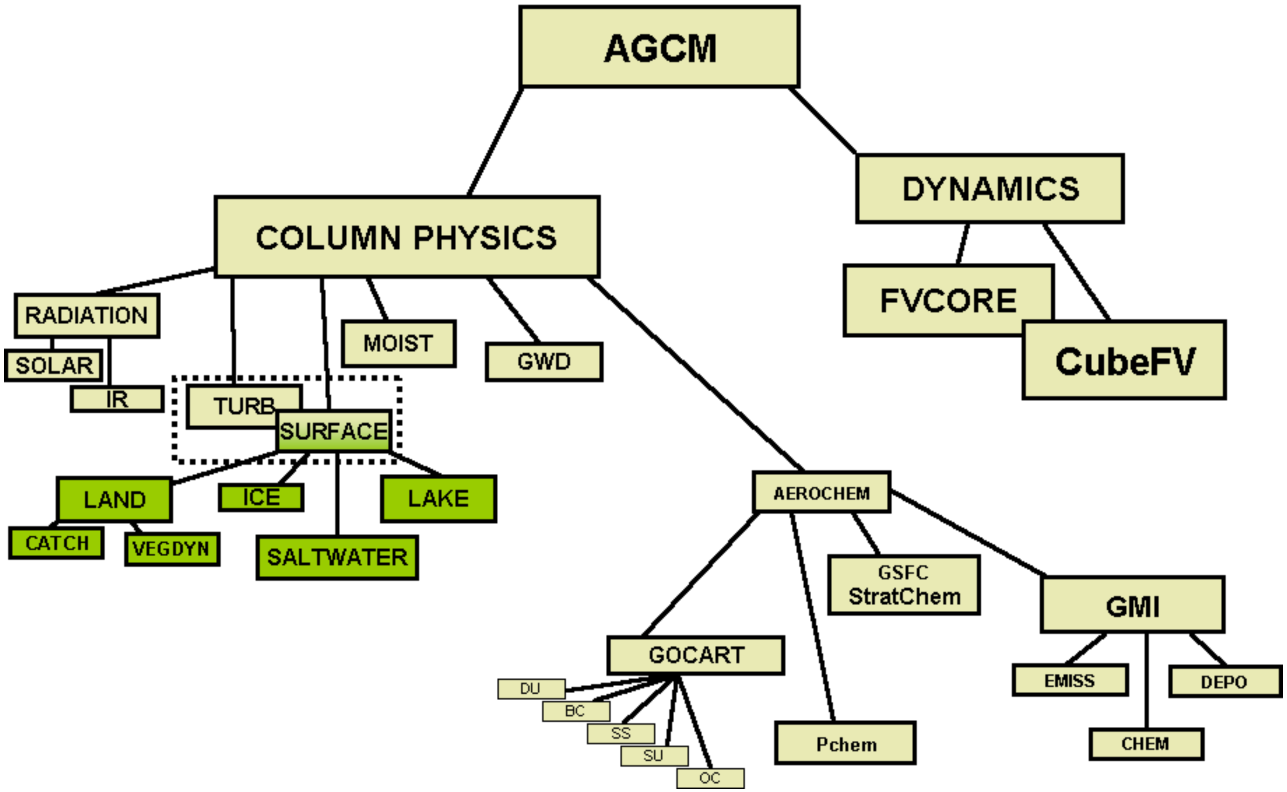
```
#ifdef _CUDA
    RUN_LOOP: do i = (blockidx%x-1)*blockdim%x+threadidx%x, &
                     ncols, blockdim%x*griddim%x
#else
    RUN_LOOP: do i = 1, ncols
#endif
        do k = 1, nlevs
          ...
```

  - Various `attributes(device)` sub-subroutines and functions
    - All levels-loop or lower! Column-loop only in main subroutine!

GPU Conversion Method

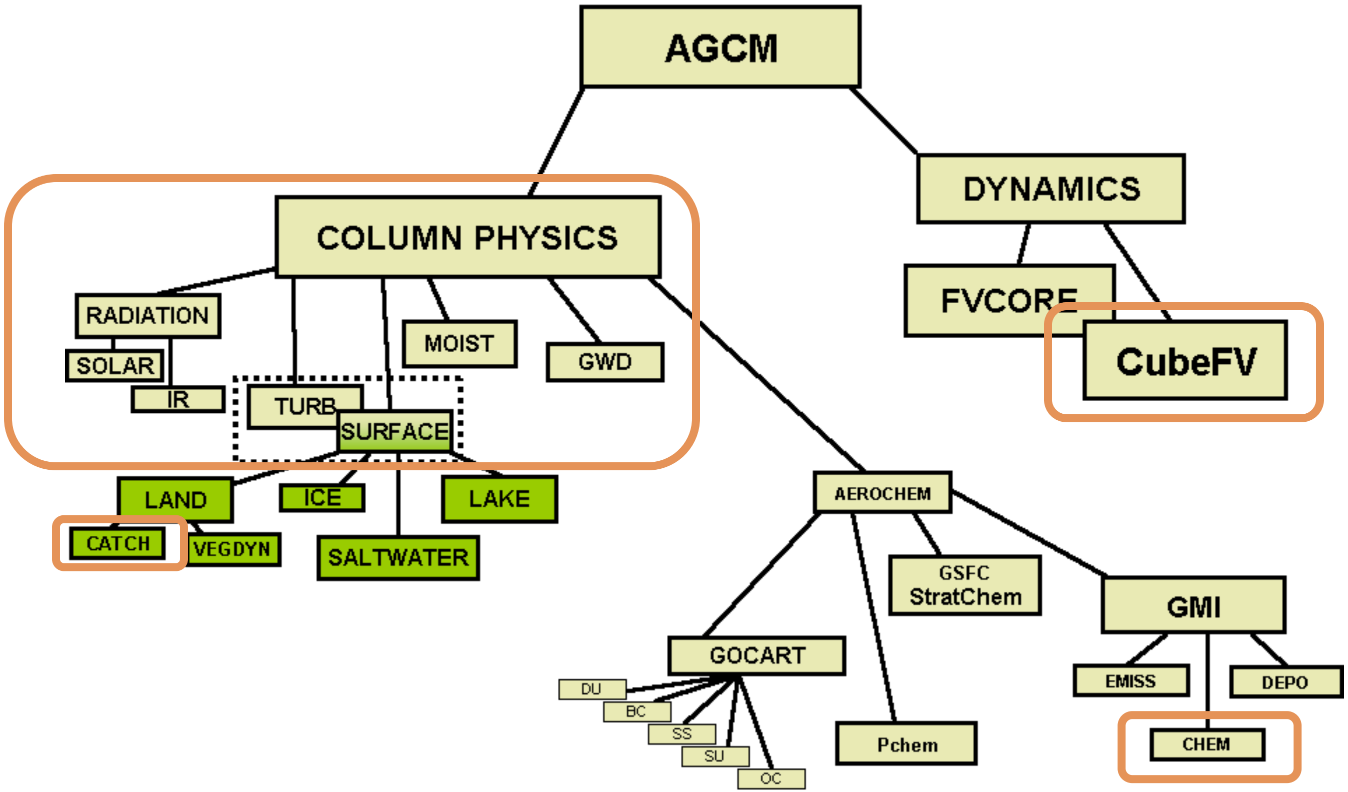
- Device Code Layout
  - Code changes mainly for memory concerns
  - Retain current procedure layout if at all possible for less impact to scientists
    - But be cruel to dead code!
  - Minimize new inputs/outputs
  - Retain all diagnostic capability

GEOS-5 GCM

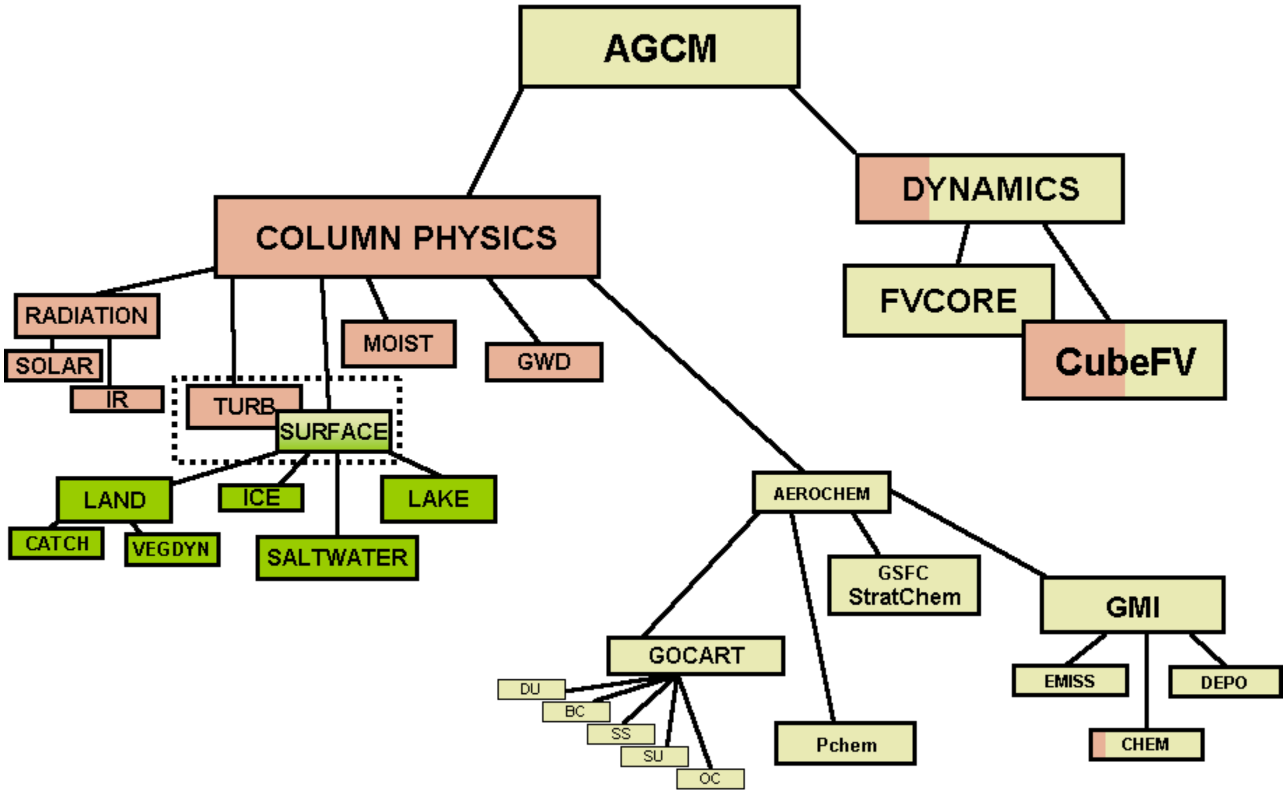


AGCM
DYNAMICS
FVCORE
CubeFV
COLUMN PHYSICS
RADIATION
SOLAR
IR
MOIST
GWD
TURB
SURFACE
LAND
ICE
LAKE
CATCH
VEGDYN
SALTWATER
AEROCHEM
GSFC StratChem
GMI
GOCART
DU
BC
SS
SU
OC
Pchem
EMISS
DEPO
CHEM

GEOS-5 GCM Targets



GEOS-5 GCM Converted



Results – Physics Kernels

Kernel	Speedup (v. Socket)
GWD	14.7x
TURBULENCE	16.7x
RAS	2.3x
CLOUD	14.7x
IRRAD	7.0x / 9.5x
SORAD	9.2x / 14.6x

Only computation (no data transfer)

System: 24 Nodes, 1 CPU (6-core X5670), 1 GPU (M2090)
Model Run: 2 Days, ½-Degree

Results – Physics Kernels

Kernel	Speedup (v. Socket)
GWD	2.6x
TURBULENCE	1.3x
RAS	1.3x
CLOUD	2.4x
IRRAD	6.4x / 8.4x
SORAD	7.9x / 11.1x

Includes allocation, deallocation, and data transfer times.

System: 24 Nodes, 1 CPU (6-core X5670), 1 GPU (M2090)
Model Run: 2 Days, ½-Degree

Results – Full Gridded Components

Gridded Component	Speedup (v. Socket)
GWD	2.6x
TURBULENCE	0.8x
MOIST	1.0x
RADIATION	1.7x / 1.7x
PHYSICS	0.9x
GCM	0.5x

Includes cost of all host code pre- and post-GPU

System: 24 Nodes, 1 CPU (6-core X5670), 1 GPU (M2090)
Model Run: 2 Days, ½-Degree

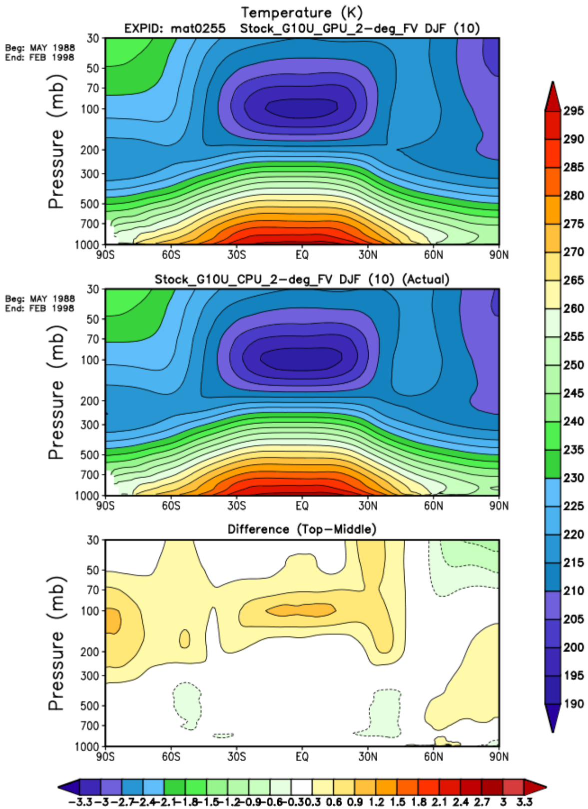
Successes – Radiation

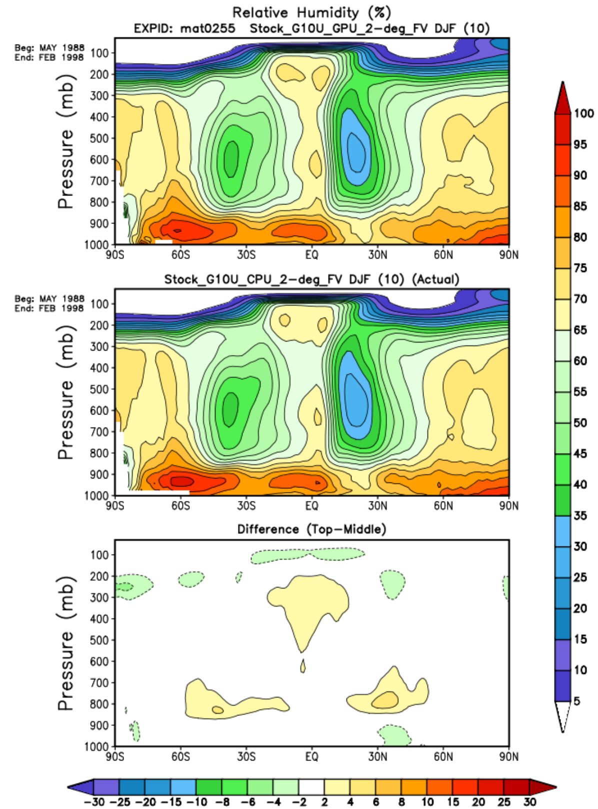
- Radiation codes are significantly faster; could allow us to do new science
  - Currently: Calculate fluxes every hour at lower resolutions, every half-hour at higher while dynamics (and all other physics) runs as often as every 3 minutes!
  - Future: Calculate fluxes every time step at all resolutions

Successes – Cloud

- Expensive cloud physics code faster as well
  - Exploiting will require careful thought to reduce data transfer costs
    - Investigate moving some calculations *back* to CPU if it reduces data transfer?

Successes – Climate





Ten-Year Climate Run at 2-degrees

DJF Zonal Mean

Left - Temp

Right - RH

Challenges – Highly Branched Code

- RAS scheme:
  - …is highly branched
    - Up to 7 levels of nested if's
  - …has different amounts of work by design
    - Some clouds are high, some are low; all columns can be different and have different path
  - Possible Solution
    - Sort columns based on return codes from previous time steps
    - Hope is that columns with similar physical characteristics have similar code paths, so warps take same path

Challenges – Many Outputs & Diagnostics

- Cloud & Turbulence tens of outputs and diagnostics
  - Allocating 50+ large 3D arrays and associated memcpys are expensive
    - In Turb: Runtime is ~10% of overall time, rest allocs and moves
  - Possible Solution
    - Test if diagnostic is needed before copying
    - Pro: Reduces data transfer time
    - Con: Code gets uglier with extra tests everywhere
    - Con: The "default" run setup exports nearly all diagnostics, and most people run that default setup to get useful data

Challenges – Using Streams

- All code still uses Stream Zero, losing out on advantages of multiple streams
  - E.g., Asynchronous data and kernel overlapping
- Why still Stream Zero?
  - Cost of allocating pinned memory currently obviates any help streams could provide
  - Might have to revisit with Kepler

Challenges – Code Readability

- CUDA Fortran code is ugly and intrusive
  - ...especially how GEOS-5 implements it
- Valid complaints from other developers
  - `#ifdef` extravaganza
  - Add to CPU code -> Add to GPU code
    - Usually means "Call Matt"
    - Slows down work
  - Interfaces can be different due to CUDA limitations
    - Might be less important with CUDA 4.0
- Possible cleanup schemes can make code more unreadable!

Challenges – Code Readability

- Managed Heap

```
ALLOCATE(Vars2d(num2dvars))
n_temp = 1
_MEMCPY(Vars2d(n_temp), temp, size(temp))
_CALL(kernel) (n_cols…)
_MEMCPY(temp, Vars2d(n_temp), size(temp))
DEALLOCATE(Vars2d)
```

Challenges – Code Readability

- Managed Heap
  - Pro: One heap allows data to stay resident on GPU longest
  - Pro: Using macros, can construct a code that is nearly CPU/GPU agnostic
    - _MEMCPY maps to either cudaMemcpy or a "cpuMemcpy" call
  - Con: Opaque (like a brick wall) to all but a few
  - Con: Requires a consistent memory placement scheme that must be adhered to rigidly
    - Slot 1 is Temperature, Slot 2 is Pressure, &c.

Challenges – Code Readability

- F2003 ASSOCIATE Block

```
#ifdef _CUDA
```

  - Allocate Device Memory
  - Memory Copies to Device

```
    ASSOCIATE(t=>t_dev, u=>u_dev…)
#endif
_CALL (kernel1) (t,u,…)
_CALL (kernel2) (t,u,…)
#ifdef _CUDA
    END ASSOCIATE
```

  - Memory Copies to Host
  - Deallocate Device Memory

```
#endif
```

Challenges – Code Readability

- F2003 ASSOCIATE Block
  - Pro: With macros, presents a single subroutine interface to multiple kernel calls
    - Not possible before CUDA 4 for us (some interfaces have 50+ members)
  - Pro: Some have experience of EQUIVALENCE, much the same style
  - Con: Memory movement is back to being an #ifdef controlled block of cudaMemcpys before and after calls
  - Con: Might require more abstraction of CUDA variables

Challenges – Code Portability

- Most important: CUDA Fortran is not that portable!
  - If PGI drops support, trouble!
- Possible solution to all our troubles: OpenACC!
  - …but…

Future Directions – OpenACC – Pros

- OpenACC is a standard
  - Should look the same for any accelerator supported
- It's like OpenMP
  - Most scientific programmers have seen OpenMP
  - Practice/Learning for Xeon Phi
- Just pragmas that are pretty readable by others
  - copy: variables copied
  - copyin: variables just copied in

Future Directions – OpenACC – Cons

- OpenACC is not designed for large, multi-nested codes
  - Requires manual inlining…
    - Pretty much a no-go
  - …or inlining by compiler
    - Every attempt has led to ACON or other compiler errors
    - GEOS-5 might require a dedicated PGI engineer just to solve these!
- Lack of memory control (tables in constant memory) could reduce performance gains
  - But by how much?

Future Directions – OpenACC

- Try conversion of working CUDA Fortran kernel to OpenACC
  - Work with PGI on one, maybe solve issues with others
- We know the data movement, so pragmas should be easy to write

Future Directions – Kepler & CUDA 5

- Our code is highly MPI decomposed so Hyper-Q might be quite helpful
  - At present can only run one core per GPU
- Big kernels mean register spilling galore at present
- Dynamic Parallelism
  - Possible boon for RAS?
- CUDA Libraries
  - Shared code (e.g., saturation specific humidity in both Turb and Cloud) in a library prevents duplication of interfaces

Future Directions – Xeon Phi

- Our code is highly MPI decomposed so native mode could be interesting
- OpenACC attempts will inform the OpenMP for Xeon Phi
- MKL on a Xeon Phi could be worth exploring
- Questions
  - Enough memory on a Xeon Phi for a full native model?
  - Data traffic is still data traffic
  - Are the memory/loop optimizations done for CUDA bad for Xeon Phi (big loops usually aren't vectorizer friendly…?)

Thanks

- Max Suarez
- Bill Putman
- GMAO, NCCS, and NAS Computing Support
- PGI Support

Questions? Suggestions?